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Stefanie Braun *, Anna-Margarete Sändig †

Abstract

We discuss whether GRIFFITH's fracture criterion for elastic bodies is also applicable to piezoelectric materials where mechanical and electric fields interact. The key point is to consider an appropriate total potential energy which reflects fracture to be a mechanical process and regards the influence of electric and mechanical loads. Furthermore, the existence of an energy minimum in the configurations has to be assured in order to characterise when a crack is stationary. This last property admits a reformulation of the GRIFFITH criterion in terms of the energy release rate, which can be expressed as a volume integral (GRIFFITH formula) or a path integral (J-integral). Starting from the well known linear VOIGT model we analyse whether the enthalpy functional (electric GIBBS energy), which is often used as the total energy functional, satisfies the above conditions. The answer is negative, i.e., due to the nonconvexity of the enthalpy density the existence of a minimiser cannot be assured. Therefore, we suggest to take the positive definite part of the enthalpy functional. This leads to an additional constitutive law, namely a linear relation between strain and electric field, which means that higher order piezo feedback is neglected. The resulting energy functional is a modified HELMHOLTZ free energy, for which the energy release rate can be mathematically rigorous expressed by a volume or path integral.

Keywords: piezoelectric materials; fracture criterion; variational methods; linear Voigt model

AMS Subject Classification: 35J50, 35E10, 74G65, 74F99

1 Introduction

Piezoelectric ceramics have widely been used as actuation devices due to intrinsic coupling effects between mechanical and electric fields. The so-called direct piezoelectric effect implies that some electric charge is induced in the piezoelectric material under mechanical load. Conversely, if some electric charge is imposed, the material reacts with mechanical deformation. Well known examples for such ceramics are lead-titanate-circonate (PZT) and barium-titanate (BT).

Piezoceramics belong to the class of brittle materials and exhibit brittle fracture behaviour. They are mathematically described by a coupled system of linear partial differential equations of second order with a generalized HOOKE's law. It is well known how the solutions (mechanical displacements and electric potentials) of this linear elliptic system of partial differential

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equations behave in a neighbourhood of a crack [3, 4]. Considering weak (variational) formulations of these equations, one gets corresponding energy functionals. But one faces certain problems as there exist different weak formulations leading to different energy functionals:

- **Skew-symmetric formulation.** The resulting energy is HELMHOLTZ's free energy:

$$E_{Helm} = \frac{1}{2} \int_{\Omega} c\varepsilon \cdot \varepsilon + \epsilon \nabla\varphi \cdot \nabla\varphi \, dx. \tag{1}$$

  Here, ε denotes the strain, φ the electric potential, c the elasticity tensor, ϵ the electrical tensor.

- **Symmetric formulation.** The resulting energy is the enthalpy:

$$E_{enth} = \int_{\Omega} \frac{1}{2} c\varepsilon \cdot \varepsilon - \frac{1}{2} \epsilon \nabla\varphi \cdot \nabla\varphi + e\varepsilon \cdot \nabla\varphi \, dx. \tag{2}$$

  Here, e is the piezo-electric material tensor, the sign '$\cdot$' denotes the corresponding scalar product.

The GRIFFITH fracture criterion in elastic materials can be formulated [6, 2] as follows: *A crack is stationary, if the total potential energy in the current configuration is minimal compared to the potential energy of all neighbouring configurations.* The existence of an energy minimiser is assumed a priori. The above energies (1),(2) have some drawbacks: On one hand, in HELMHOLTZ's free energy (1) the piezoelectric coupling of the system is neglected and the corresponding EULER-LAGRANGE equations do not completely coincide with the considered coupled piezoelectric system. Thus, a weak solution of the piezoelectric system is not necessaryly a minimiser of HELMHOLTZ's free energy. On the other hand, the enthalpy density in (2) is not convex and the existence of a minimizer cannot be assured.
To get over these disadvantages, we consider only the positive definite part of the enthalpy density. This may presumably cover the leading part, as the negative eigenvalues are quite small compared to the positive ones. Consequently, the field equations simplify and the HELMHOLTZ free energy is considered together with an additional condition expressing the linear coupling between mechanical strain and electric field:

$$E_{Helm} = \frac{1}{2} \int_{\Omega} c\varepsilon \cdot \varepsilon + \epsilon \nabla\varphi \cdot \nabla\varphi \, dx, \quad \nabla\varphi = \epsilon^{-1} e\varepsilon. \tag{3}$$

Thus, one gets a modified elastic energy. The mechanial character of the fracture process is preserved. The corresponding weak boundary value problem for the EULER-LAGRANGE equations has a unique solution reflecting the mechanical and electric loads. Moreover, this solution is a minimiser of the modified HELMHOLTZ free energy. These properties allow to reformulate GRIFFITH's fracture criterion in terms of the energy release rate. The computation of the energy release rate can be carried out based on a volume integral (GRIFFITH formula) or a path integral (J-integral). Furthermore, it is possible to derive formulas expressing the energy release rate in the form of stress intensity factors.
Let us mention there are other fracture criteria used in mechanics for piezoelectric ceramics, e.g. [8, 9, 10, 5].

2 Linear piezoelectric field equations

Characterised by three different interacting physical systems of fields, namely elastic, electric and thermo-dynamic fields, piezoelectricity is a rather complex phenomenon. A widely used model for describing the electro-mechanical coupling effect is the so-called linear VOIGT-model which allows a comparatively easy mathematical handling by omitting complicated hysteresis effects. In the following section this model shall be derived and thereafter used for setting up a boundary value problem describing a piezoelectric ceramic exposed to an external electric voltage.
Starting with the electric system and its set of independent variables, namely the electric field strength E and the dielectric displacement D, one can assume the electric field to be quasi-static, i.e. the electric field strength can be expressed as a vector potential $E = -\nabla\varphi$. In the absence of electro-mechanical coupling the relation between electric field strength and displacement can be written as $D = \epsilon_0 E + P$, where ϵ_0 is the absolute permittivity and P the polarisation of the material. Assuming the relationship between polarisation and electric field strength to be linear, this equation reads $D_i = \epsilon_{ij}E_j$ and accordingly $E_i = \beta_{ij}D_j$, where ϵ now is the relative permittivity tensor and β the dielectric impermeability. Here and in the following EINSTEIN's sum convention is used.
Another crucial relation for the piezoelectric field equations derives from one of Maxwell's macroscopic equations, namely Gauss's law:

$$\mathrm{div}D = \rho_e.$$

Neglecting the external load density ρ_e one gains

$$\mathrm{div}D = 0. \tag{4}$$

This equation will be one of the two differential equations building the later formulated boundary value problem.
The second of the differential equations can be derived from the mechanical system: independent variables of this system are mechanical stress σ and strain ε, where ε represents the symmetric part of the displacement field u, $\varepsilon_{ij} = \frac{1}{2}(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j})$. In linear elasticity the relation between stress and strain is expressed by HOOKE's law

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} \qquad \text{or} \qquad \varepsilon_{ij} = s_{ijkl}\sigma_{kl}$$

with elastic stiffness and elastic compliance c and s, respectively. CAUCHY's stress principle provides general equilibrum conditions

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_{b_i} = 0. \tag{5}$$

Once again neglecting external body forces f_{b_i} and introducing the generalised matrix divergence operator $\mathrm{Div} = \begin{pmatrix} \frac{\partial}{\partial x_1} & 0 & 0 \\ 0 & \frac{\partial}{\partial x_2} & 0 \\ 0 & 0 & \frac{\partial}{\partial x_3} \\ \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1} & 0 \\ 0 & \frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} & 0 & \frac{\partial}{\partial x_1} \end{pmatrix}$, equation (5) reads

$$\mathrm{Div}^T\sigma = 0. \tag{6}$$

Conservation of the angular momentum yields the symmetry of the stress tensor σ.

The third and so far not considered thermodynamic system possesses again a set of two new independent variables, temperature T and entropy S. However, as for this paper temperature dependence of the piezoelectric effect shall be neglected, both temperature and entropy will not appear in any of the modelling equations. The thermodynamic system is nonetheless of great importance for the model as it is used for explicitely deriving the piezoelectric field equations on the basis of a thermodynamic potential. Choosing e.g. the electric enthalpy

$$H = U - E \cdot D,$$

where U represents the internal energy of the system, and building the time derivative one gets

$$\dot{H} = \dot{U} - E \cdot \dot{D} - \dot{E} \cdot D. \tag{7}$$

With the first law of thermodynamics

$$dU = dW + dQ,$$

describing the change in the internal energy of a closed thermodynamic system as the sum of the amount of heat energy Q supplied to the system and the work W done to the system, and the term for piezoelectric work

$$dW = \sigma_{ij} d\varepsilon_{ij} + E_i dD_i$$

equation (7) reads

$$\dot{H} = \sigma_{ij}\dot{\varepsilon}_{ij} - D_i \cdot \dot{E}_i.$$

On the other hand, by building the total time derivative of the enthalpy $H = H(\varepsilon, E)$ one gets

$$\dot{H} = \frac{\partial H}{\partial \varepsilon_{ij}}\dot{\varepsilon}_{ij} + \frac{\partial H}{\partial E_i}\dot{E}_i$$

and consequently

$$\sigma_{ij} = \frac{\partial H}{\partial \varepsilon_{ij}} \qquad \text{and} \qquad D_i = -\frac{\partial H}{\partial E_i}. \tag{8}$$

by comparison of the coefficients.

Stress $\sigma = \sigma(\varepsilon, E)$ and dielectric displacement $D = D(\varepsilon, E)$ can now be expanded into a first-order Taylor series approximation about some constant fields $\sigma^0_{ij} = \sigma_{ij}(\varepsilon^0_{kl}, E^0_k)$ and $D^0_i = D_i(\varepsilon^0_{kl}, E^0_k)$:

$$\begin{aligned}
\sigma_{ij} &\approx \sigma_{ij}(\varepsilon^0_{kl}, E^0_k) + \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}}(\varepsilon_{kl} - \varepsilon^0_{kl}) + \frac{\partial \sigma_{ij}}{\partial E_k}(E_k - E^0_k) \\
D_i &\approx D_i(\varepsilon^0_{kl}, E^0_k) + \frac{\partial D_i}{\partial \varepsilon_{kl}}(\varepsilon_{kl} - \varepsilon^0_{kl}) + \frac{\partial D_i}{\partial E_k}(E_k - E^0_k).
\end{aligned}$$

In the absence of impressed residual stresses in the material, the quantities σ^0_{ij} and D^0_i as well ε^0_{kl} and E^0_k can be set 0 without loss of generality. Restricting to the linear model, we assume

$$\sigma_{ij} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}}\varepsilon_{kl} + \frac{\partial \sigma_{ij}}{\partial E_k}E_k \tag{9}$$

$$D_i = \frac{\partial D_i}{\partial \varepsilon_{kl}}\varepsilon_{kl} + \frac{\partial D_i}{\partial E_k}E_k. \tag{10}$$

Inserting (8) into equations (9),(10) yields

$$\begin{aligned} \sigma_{ij} &= \underbrace{\frac{\partial^2 H}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}}}_{c_{ijkl}}\varepsilon_{kl} + \underbrace{\frac{\partial^2 H}{\partial \varepsilon_{ij}\partial E_k}}_{-e_{ijk}}E_k \\ D_i &= \underbrace{-\frac{\partial^2 H}{\partial E_i\partial \varepsilon_{kl}}}_{e_{ikl}}\varepsilon_{kl} \underbrace{-\frac{\partial^2 H}{\partial E_i\partial E_k}}_{\epsilon_{ik}}E_k, \end{aligned}$$

which leads to the following definition of the material parameters:

$$\begin{aligned} c_{ijkl} &= \frac{\partial^2 H}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}} \\ e_{ikl} &= -\frac{\partial^2 H}{\partial E_i\partial \varepsilon_{kl}} = -\frac{\partial \sigma_{kl}}{\partial E_i} = \frac{\partial D_i}{\partial \varepsilon_{kl}} \\ \epsilon_{ik} &= -\frac{\partial^2 H}{\partial E_i\partial E_k} = \frac{\partial D_i}{\partial E_k}. \end{aligned}$$

With the use of these abbreviations the constitutive field equations for piezoelectric materials read

$$\sigma = c\varepsilon - eE, \tag{11}$$

$$D = e\varepsilon + \epsilon E. \tag{12}$$

The tensors c and ϵ represent again elastic stiffness and electric permittivity, respectively, whereas e is the piezoelectric tensor.

Remark 2.1. Having regard to the order of the differentiation, two different piezoelectric tensors appear:

$$e_{ikl_1} = -\frac{\partial \sigma_{ij}}{\partial E_k} = \frac{\partial^2 H}{\partial \varepsilon_{ij}\partial E_k} \qquad \text{and} \qquad e_{ikl_2} = \frac{\partial D_i}{\partial \varepsilon_{kl}} = \frac{\partial^2 H}{\partial E_i\partial \varepsilon_{kl}}.$$

However, as one of them represents the constant for the direct piezoelectric effect whereas the other gives the constant for the inverse effect, one can show that they coincide.

In the following, for the purpose of clarity VOIGT index notation shall be used, which allows to express the constitutive laws in a matrix-vector-form as the material tensors can be written as matrices. To further simplify the notation, the elastic, piezoelectric and electric material matrices are combined to the skewsymmetric material matrix

$$A = \begin{pmatrix} c & -e^T \\ e & \epsilon \end{pmatrix},$$

with the help of which the constitutive laws can be written in the following form

$$\begin{pmatrix} \sigma \\ D \end{pmatrix} = A \begin{pmatrix} \varepsilon \\ E \end{pmatrix}.$$

For the purpose of reducing the three-dimensional problem to a two-dimensional one, the considered piezoelectric material is considered to be in a plane-strain-state, i.e. the material is isotropic in the $x_1 - x_2-$plane, whereas the polarisation axis coincides with the x_3-axis. Reducing the problem to the $x_1 - x_3-$plane, one gains the additional conditions

$$\begin{aligned} \varepsilon_{21} = \varepsilon_{22} = \varepsilon_{23} &= 0 \\ E_2 &= 0 \\ \varphi &= \varphi(x_1, x_3) \\ u_i &= u_i(x_1, x_3),\ i = 1, 3, u_2 = 0. \end{aligned}$$

Furthermore, the material parameters are assumed to be independent of x_2. With these simplifications one gets the following set of constitutive equations

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{33} \\ \sigma_{13} \\ D_1 \\ D_3 \end{pmatrix} = \begin{bmatrix} c_{11} & c_{13} & 0 & 0 & -e_{31} \\ c_{13} & c_{33} & 0 & 0 & -e_{33} \\ 0 & 0 & c_{44} & -e_{15} & 0 \\ 0 & 0 & e_{15} & \epsilon_{11} & 0 \\ e_{31} & e_{33} & 0 & 0 & \epsilon_{33} \end{bmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{33} \\ 2\varepsilon_{13} \\ E_1 \\ E_3 \end{pmatrix}. \tag{13}$$

3 The boundary value problem in the cracked domain

Figure 1 shows a cylindrical piece of a transversal isotropic ceramic with a pre-existing two-dimensional crack perpendicular to the polar axis.

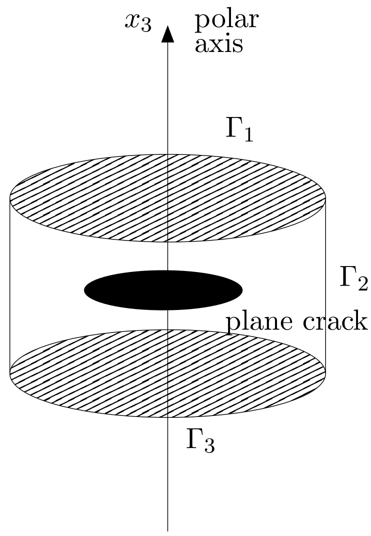

Figure 1: Piece of ceramic

To reduce the problem to plane-strain-state, one takes a look only at a cross-section of the ceramic. As the crack propagation is assumed to take place only in the crack plane, in the two-dimensional case the crack only propagates along the (positive) x_1-axis. The coordinate system may be chosen in such a way that the crack starts at $x_3 = 0$.

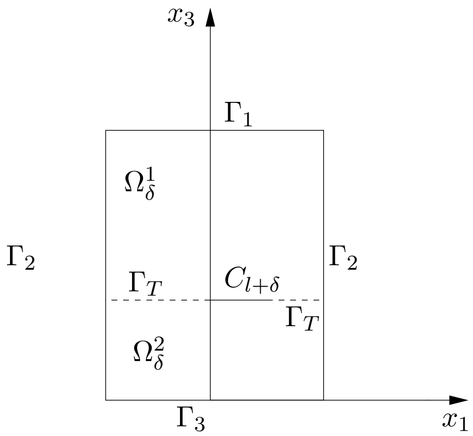

Figure 2: Ceramic in plane-strain-state

Definition 3.1. Let $\Omega \in \mathbb{R}^2$ be an open set in the above mentioned cross-section which fully contains the crack $C_l = \{(x_1, x_3 = 0) : 0 < x_1 < l\}$, and $\Omega_0 = \Omega\backslash C_l$ the set with a crack. Likewise, for $\delta > 0$, let $C_{l+\delta} = \{(x_1, x_3 = 0) : 0 < x_1 < l + \delta\}$ and $\Omega_\delta = \Omega\backslash C_{l+\delta}$, describing a set with a crack that has elongated by δ.

We want to use certain inequalities and estimations demanding that the boundary of the domain under consideration satisfies a Lipschitz condition, which is not the case for a domain containing a crack. Therefore, we introduce formally an interface Γ_T deviding the domain $\overline{\Omega_\delta}$ into two parts $\overline{\Omega^1_\delta}$ and $\overline{\Omega^2_\delta}$ with $\Omega^1_\delta \cap \Omega^2_\delta = C_{l+\delta} \cup \Gamma_T$, see Figure 2, and demand that both subdomains are Lipschitz domains.

Definition 3.2. Let $\overline{\Omega}_\delta = \overline{\Omega^1}_\delta \cup \overline{\Omega^2}_\delta$ for $\delta \in [0, a]$ and $\Omega^1_\delta \cap \Omega^2_\delta = \emptyset$, where Ω^1_δ and Ω^2_δ denote open and connected sets. The crack faces are given by $C^j_{l+\delta} = \partial\Omega^j_\delta \cap C_{l+\delta}$, $j = 1, 2$.

Consider now the ceramic to have a clamped support at the bottom side Γ_3, whereas all other sides shall remain unclamped such that the ceramic can freely expand or contract due to the piezoelectric effect when an electric voltage is impressed between top Γ_1 and bottom Γ_3.

To formulate the boundary value problem we start from the differential equations (4, 6) which are coupled by the constitutive relations (11, 12):

$$\mathrm{Div}^\top(c\varepsilon - eE) = 0 \tag{14}$$
$$\mathrm{div}\,(e\varepsilon + \epsilon E) = 0. \tag{15}$$

In order to simplify the notation the generalised displacement vector is introduced:

$$U := \begin{pmatrix} u \\ \varphi \end{pmatrix}$$

In this notation the two differential equations can easily be expressed as

$$-\mathcal{B}^T A \mathcal{B} U = 0, \tag{16}$$

$$\mathcal{B} := \begin{pmatrix} \partial_1 & 0 & 0 \\ 0 & \partial_3 & 0 \\ \partial_3 & \partial_1 & 0 \\ 0 & 0 & -\partial_1 \\ 0 & 0 & -\partial_3 \end{pmatrix}.$$

We study the following transmission-boundary value problem:

$$\begin{aligned} -\mathcal{B}^T A \mathcal{B} U_j &= 0 && \text{in} \quad \Omega_\delta^j \\ u_2 &= 0 && \text{on} \quad \Gamma_m^D = \Gamma_3 \\ \varphi_j &= \pm\varphi_a && \text{on} \quad \Gamma_e^{D,j} = (\Gamma_1 \cup \Gamma_3) \cap \partial\Omega_\delta^j \\ \sigma_{n_j} = N_j^T \left(c\varepsilon(u_j) + e^T \nabla\varphi_j \right) &= 0 && \text{on} \quad \Gamma_m^{N,j} = (\Gamma_1 \cup \Gamma_2) \cap \partial\Omega_\delta^j \\ D_{n_j} = n_j^T (e\varepsilon(u_j) - \epsilon\nabla\varphi_j) &= 0 && \text{on} \quad \Gamma_e^{N,j} = \Gamma_2 \cap \partial\Omega_\delta^j \\ \sigma_{n_j} = D_{n_j} &= 0 && \text{on} \quad C_{l+\delta}^j \\ u_1 = u_2, \quad \varphi_1 &= \varphi_2 && \text{on} \quad \Gamma_T \\ N_1^T \left(c\varepsilon(u_1) + e^T \nabla\varphi_1 \right) + N_2^T \left(c\varepsilon(u_2) + e^T \nabla\varphi_2 \right) &= 0 && \text{on} \quad \Gamma_T \\ n_1^T (e\varepsilon(u_1) - \epsilon\nabla\varphi_1) + n_2^T (e\varepsilon(u_2) - \epsilon\nabla\varphi_2) &= 0 && \text{on} \quad \Gamma_T. \end{aligned}$$

U_j denotes the restriction of U on Ω_δ^j, σ_{n_j} and D_{n_j} are the normal stresses and normal displacements, respectively; N_j denotes the generalised normal operator, $j = 1, 2$.

$$N_j = \begin{pmatrix} n_{1,j} & 0 \\ 0 & n_{3,j} \\ n_{3,j} & n_{1,j} \end{pmatrix}.$$

This transmission-boundary value problem can be formulated shorter as boundary value problem in the cracked domain Ω_δ:

$$-\mathcal{B}^T A \mathcal{B} U = 0 \quad \text{in} \quad \Omega_\delta \tag{17}$$
$$u = 0 \quad \text{on} \quad \Gamma_m^D = \Gamma_3 \tag{18}$$
$$\varphi = \pm\varphi_a \quad \text{on} \quad \Gamma_e^D = \Gamma_1 \cup \Gamma_3 \tag{19}$$
$$\sigma_n = N^T \left(c\varepsilon(u) + e^T \nabla\varphi \right) = 0 \quad \text{on} \quad \Gamma_m^N = \Gamma_1 \cup \Gamma_2 \tag{20}$$
$$D_n = n^T (e\varepsilon(u) - \epsilon\nabla\varphi) = 0 \quad \text{on} \quad \Gamma_e^N = \Gamma_2 \tag{21}$$
$$\sigma_{n_j} = 0, \; D_{n_j} = 0 \quad \text{on} \quad C_{l+\delta}, \; j = 1, 2. \tag{22}$$

Note that the subscripts m and e describe mechanical and electric boundary conditions, respectively, whereas the superscripts D and N denote Dirichlet or Neumann boundary conditions, respectively.

4 Weak formulations

Based on the boundary value problem (17,18,19,20,21,22) one can derive two different weak formulations with various properties, corresponding to two different energy functionals. Both formulations and their properties shall be discussed.

4.1 Skew-symmetric formulation

At first, we introduce classical Sobolev spaces in which we look for weak solutions. Let

$$H^1(\Omega_\delta) = \{u \in L_2(\Omega_\delta) : \|u\|^2_{H^1(\Omega_\delta)} = \int_{\Omega_\delta} |u|^2\,dx + \sum_{i=1,2} \int_{\Omega_\delta} |\frac{\partial u}{\partial x_i}|^2\,dx < \infty\}.$$

Remark 4.1. Note that $\int\limits_{\Omega_\delta}$ shall always denote the sum of the two integrals $\int\limits_{\Omega^1_\delta}$ and $\int\limits_{\Omega^2_\delta}$.

For the generalized vector $V = \begin{pmatrix} v \\ \psi \end{pmatrix}$ we consider an appropriate subspace, where the homogeneous Dirichlet conditions are realized:

$$\mathcal{V}_\delta := \{V = \begin{pmatrix} v \\ \psi \end{pmatrix} \in [H^1(\Omega_\delta)]^3 : v|_{\Gamma^D_m} = 0,\ \ \psi|_{\Gamma^D_e} = 0\}, \qquad \delta \in [0, a]. \tag{23}$$

Multiplying equation (17) by a test function $V = \begin{pmatrix} v \\ \psi \end{pmatrix} \in \mathcal{V}_\delta$ and integrating by parts leads to

$$\begin{aligned}
-\int\limits_{\Omega_\delta} \mathcal{B}^T A\mathcal{B}U \cdot V\,dx &= -\int\limits_{\Omega^1_\delta} \mathcal{B}^T A\mathcal{B}U_1 \cdot V_1\,dx - \int\limits_{\Omega^2_\delta} \mathcal{B}^T A\mathcal{B}U_2 \cdot V_2\,dx \\
&= \int\limits_{\Omega^1_\delta} A\mathcal{B}U_1 \cdot \mathcal{B}V_1 dx - \int\limits_{\partial\Omega^1_\delta} N_1^T A\mathcal{B}U_1 \cdot V_1\,da \\
&\quad + \int\limits_{\Omega^2_\delta} A\mathcal{B}U_2 \cdot \mathcal{B}V_2\,dx - \int\limits_{\partial\Omega^2_\delta} N_2^T A\mathcal{B}U_2 \cdot V_2\,da = 0 \qquad \forall V \in \mathcal{V}_\delta.
\end{aligned}$$

Here, $U_i = U|_{\Omega^i_\delta}, V_i = V|_{\Omega^i_\delta}, i = 1, 2$.

Now, we decompose $U = U^0 + W$, where $U^0 = \begin{pmatrix} u \\ \varphi^0 \end{pmatrix} \in \mathcal{V}_\delta$ and $W = \begin{pmatrix} 0 \\ \tilde{\varphi}(x_3) \end{pmatrix}$. $\tilde{\varphi}(x_3)$ denotes a smooth continuation of the boundary charges $\pm\varphi_a$ on Γ^D_m, only depending on x_3, onto the domain $\bar{\Omega}_\delta$. Taking into account the boundary conditions, this yields

$$\int\limits_{\Omega_\delta^1} A\mathcal{B}U_1^0 \cdot \mathcal{B}V_1 dx - \int\limits_{\partial\Omega_\delta^1} N_1^T A\mathcal{B}U_1^0 \cdot V_1 da + \int\limits_{\Omega_\delta^2} A\mathcal{B}U_2^0 \cdot \mathcal{B}V_2 dx - \int\limits_{\partial\Omega_\delta^2} N_2^T A\mathcal{B}U_2^0 \cdot V_2 da$$

$$\begin{aligned}
= & \int\limits_{\Omega_\delta^1} A\mathcal{B}U_1^0 \cdot \mathcal{B}V_1 dx + \int\limits_{\Omega_\delta^2} A\mathcal{B}U_2^0 \cdot \mathcal{B}V_2 dx - \int\limits_{\Gamma_1} \underbrace{\sigma_{n_1}}_{=0} \cdot v_1 da - \int\limits_{\Gamma_2} \underbrace{\sigma_n}_{=0} \cdot v da \\
& - \int\limits_{\Gamma_3} \sigma_{n_2} \cdot \underbrace{v_2}_{=0} da - \int\limits_{\Gamma_1} D_{n_1} \cdot \underbrace{\psi_1}_{=0} da - \int\limits_{\Gamma_2} \underbrace{D_n}_{=0} \cdot \psi da - \int\limits_{\Gamma_3} D_{n_2} \cdot \underbrace{\psi_2}_{=0} da \\
& - \int\limits_{C^1_{(l+\delta)}} \underbrace{\sigma_{n_1}}_{=0} \cdot v_1 da - \int\limits_{C^2_{(l+\delta)}} \underbrace{\sigma_{n_2}}_{=0} \cdot v_2 da - \int\limits_{C^1_{(l+\delta)}} \underbrace{D_{n_1}}_{=0} \cdot \psi_1 da - \int\limits_{C^2_{(l+\delta)}} \underbrace{D_{n_2}}_{=0} \cdot \psi_2 da \\
= & \int\limits_{\Omega_\delta^1} A\mathcal{B}U_1^0 \cdot \mathcal{B}V_1 dx + \int\limits_{\Omega_\delta^2} A\mathcal{B}U_2^0 \cdot \mathcal{B}V_2 dx \\
= & - \int\limits_{\Omega_\delta^1} A\mathcal{B}W_1 \cdot \mathcal{B}V_1 dx - \int\limits_{\Omega_\delta^2} A\mathcal{B}W_2 \cdot \mathcal{B}V_2 dx \\
= & - \int\limits_{\Omega_\delta} A\mathcal{B}W \cdot \mathcal{B}V dx \qquad \forall V \in \mathcal{V}_\delta.
\end{aligned}$$

Thus, the skew-symmetric weak formulation (remind that A is skew-symmetric) reads as follows:

Find $U^0 \in \mathcal{V}_\delta$, $U^0 = U - W$, such that it holds for all $V \in \mathcal{V}_\delta$

$$a(U^0, V) := \int\limits_{\Omega_\delta} A\mathcal{B}U^0 \cdot \mathcal{B}V dx = - \int\limits_{\Omega_\delta} A\mathcal{B}W \cdot \mathcal{B}V dx =: -a(W, V), \qquad 0 \le \delta \le a. \tag{24}$$

Existence and uniqueness of a weak solution can easily be shown with the help of the Lax-Milgram theorem which holds for unsymmetric, continuous, $\mathcal{V}_\delta$-elliptic bilinear forms, too, see [1], page 60.

Theorem 4.2. *The skew-symmetric weak formulated boundary value problem (24) has a uniquely defined solution in $\mathcal{V}_\delta$.*

Proof. The boundedness (equivalent to the continuity) of the bilinear form $a(\cdot,\cdot)$ on $\mathcal{V}_\delta \times \mathcal{V}_\delta$ is obvious. To show ellipticity, consider

$$\begin{aligned}
a(V, V) &= \int\limits_{\Omega_\delta} \begin{pmatrix} c & -e^T \\ e & \epsilon \end{pmatrix} \begin{pmatrix} \varepsilon(v) \\ -\nabla\psi \end{pmatrix} \cdot \begin{pmatrix} \varepsilon(v) \\ -\nabla\psi \end{pmatrix} dx \\
&= \int\limits_{\Omega_\delta} c\varepsilon(v) \cdot \varepsilon(v) + e\varepsilon(v) \cdot \nabla\psi - e\varepsilon(v) \cdot \nabla\psi + \epsilon\nabla\psi \cdot \nabla\psi \, dx \qquad (25) \\
&= \int\limits_{\Omega_\delta} c\varepsilon(v) \cdot \varepsilon(v) + \epsilon\nabla\psi \cdot \nabla\psi \, dx.
\end{aligned}$$

As both elastic stiffness and electric permittivity are positive definite tensors, electric and mechanical part can be looked at separately and estimated by their smallest eigenvalues. The above introduced splitting of Ω_δ into the subdomains $\Omega_\delta^1, \Omega_\delta^2$ and the interface Γ_T makes it possible to apply Korn's inequality for mixed boundary value problems, see [7]. Thus we get

$$\begin{aligned} a(V,V) &\geqq c_{1,m} \parallel v \parallel^2_{[H^1(\Omega_\delta)]^2} + c_{1,e} \parallel \psi \parallel^2_{H^1(\Omega_\delta)} \\ &\geq min(c_{1,m}, c_{1,e}) \parallel V \parallel^2_{\mathcal{V}_\delta} \\ &= c_1 \parallel V \parallel^2_{\mathcal{V}_\delta} . \end{aligned}$$

□

The energy functional adjoint to the problem (24) reads

$$\begin{aligned} I = \frac{1}{2}a(U,U) + a(W,U) &= \int_{\Omega_\delta} (\frac{1}{2}c\varepsilon(u)\cdot\varepsilon(u) + \frac{1}{2}\epsilon\nabla\varphi\cdot\nabla\varphi + A\mathcal{B}W\cdot\mathcal{B}U)\,dx \quad (26) \\ &= \int_{\Omega_\delta} L(\mathcal{B}U)\,dx, \end{aligned}$$

with the Lagrange function

$$L(\mathcal{B}U) = \frac{1}{2}c\varepsilon(u)\cdot\varepsilon(u) + \frac{1}{2}\epsilon\nabla\varphi\cdot\nabla\varphi + A\mathcal{B}W\cdot\mathcal{B}U.$$

The corresponding weak Euler-Lagrange equations read

$$a^*(U,V) = \int_{\Omega_\delta} \begin{pmatrix} c & 0 \\ 0 & \epsilon \end{pmatrix} \begin{pmatrix} \varepsilon(u) \\ -\nabla\varphi \end{pmatrix} \cdot \begin{pmatrix} \varepsilon(v) \\ -\nabla\varphi \end{pmatrix} dx = -a(W,V) \quad \forall V \in \mathcal{V}_\delta. \quad (27)$$

It turns out that the uniquely defined minimizer in $\mathcal{V}_\delta$ of the energy functional (26) coincides with the uniquely defined weak solution of (27) and not with the uniquely defined weak solution of our original problem(24). Consequently, the Griffith fracture criterion applied to the energy functional (26) does not reflect the piezoelectric coupling.
Therefore, we consider a symmetric weak formulation with the enthalpy as energy functional in the following section.

Remark 4.3. The form of the energy functional I depends strongly on the choice of the admissible displacement fields.

4.2 Symmetric formulation

By trying to change the energy functional in such way that the two piezoelectric terms sum up instead of cancelling each other as in (25), one gets a new definition of the generalised displacement vector:

$$U^* = \begin{pmatrix} u \\ -\varphi \end{pmatrix}.$$

Defininig

$$\mathcal{B}^* = \begin{pmatrix} \partial_1 & 0 & 0 \\ 0 & \partial_3 & 0 \\ \partial_3 & \partial_1 & 0 \\ 0 & 0 & \partial_1 \\ 0 & 0 & \partial_3 \end{pmatrix}$$

and the symmetric matrix

$$\tilde{A} = \begin{pmatrix} c & -e^T \\ -e & -\epsilon \end{pmatrix} = \begin{pmatrix} c_{11} & c_{13} & 0 & 0 & -e_{31} \\ c_{13} & c_{33} & 0 & 0 & -e_{33} \\ 0 & 0 & c_{44} & -e_{15} & 0 \\ 0 & 0 & -e_{15} & -\epsilon_{11} & 0 \\ -e_{31} & -e_{33} & 0 & 0 & -\epsilon_{33} \end{pmatrix},$$

the coupled system of partial differential equations (17) can be written in the same form as before,

$$-\mathcal{B}^{*\top} \tilde{A} \mathcal{B}^* U^* = 0. \tag{28}$$

The boundary conditions (18–22) can be reformulated correspondingly and W goes over to W^*. Furthermore, we introduce the function space

$$\mathcal{V}_\delta{}^* := \{V = \begin{pmatrix} v \\ -\psi \end{pmatrix} \in [H^1(\Omega_\delta)]^3 : v|_{\Gamma_m^D} = 0, \;\; \psi|_{\Gamma_e^D} = 0\}, \qquad \delta \in [0, a]. \tag{29}$$

In the same way as we have derived (24) we come to the weak symmetric formulation:
Find $U^{0^*} \in \mathcal{V}_\delta{}^*$, $U^{0^*} = U^* - W^*$, *such that it holds for all* $V^* \in \mathcal{V}_\delta{}^*$

$$\tilde{a}(U^{0^*}, V^*) \;:=\; \int_{\Omega_\delta} \tilde{A}\mathcal{B}^* U^{0^*} \cdot \mathcal{B}^* V^* dx = -\int_{\Omega_\delta} \tilde{A}\mathcal{B}^* W^* \cdot \mathcal{B}^* V^* dx =: -\tilde{a}(W^*, V^*), \quad 0 \le \delta \le a.$$

Note that

$$\int_{\Omega_\delta} \tilde{A}\mathcal{B}^* U^{0^*} \cdot \mathcal{B}^* V^* dx = \int_{\Omega_\delta} (c\varepsilon(u) \cdot \varepsilon(v) + e\varepsilon(u) \cdot \nabla\psi + e\varepsilon(v)\nabla\varphi^0 - \epsilon\nabla\varphi^0 \cdot \nabla\psi)\, dx. \tag{30}$$

Unfortunately, we cannot guarantee that a uniquely defined weak solution of (30) exists, since the bilinear form $\tilde{a}(\cdot,\cdot)$ on $\mathcal{V}_\delta{}^* \times \mathcal{V}_\delta{}^*$ is not elliptic (the matrix $\tilde{A}$ is not positive definite) and therefore the Lax-Milgram theorem is not applicable.

Nevertheless, we can introduce formally the adjoint energy functional

$$I = \frac{1}{2}\tilde{a}(U^*, U^*) + \tilde{a}(W^*, U^*) \tag{31}$$

$$= \int_{\Omega_\delta} (\frac{1}{2} c\varepsilon(u) \cdot \varepsilon(u) + e\varepsilon(u) \cdot \nabla\varphi - \frac{1}{2}\epsilon\nabla\varphi \cdot \nabla\varphi + \tilde{A}\mathcal{B}^* W^* \cdot \mathcal{B}^* U^*)\, dx \tag{32}$$

$$= \int_{\Omega_\delta} L^*(\mathcal{B}^* U^*)\, dx, \tag{33}$$

The LAGRANGE function is here

$$
\begin{aligned}
L^*(\mathcal{B}^*U^*) &= \frac{1}{2}\sigma\cdot\varepsilon - \frac{1}{2}E\cdot D + \mathcal{B}^*W^*\cdot\mathcal{B}^*U^* && (34)\\
&= \frac{1}{2}c\varepsilon(u)\cdot\varepsilon(u) + e\varepsilon(u)\cdot\nabla\varphi - \frac{1}{2}\epsilon\nabla\varphi\cdot\nabla\varphi + \mathcal{B}^*W^*\cdot\mathcal{B}^*U^* && (35)\\
&= H + \mathcal{B}^*W^*\cdot\mathcal{B}^*U^*, && (36)
\end{aligned}
$$

where

$$
\begin{aligned}
H &:= \frac{1}{2}\sigma\cdot\varepsilon - \frac{1}{2}E\cdot D\\
&= \frac{1}{2}c\varepsilon(u)\cdot\varepsilon(u) + e\varepsilon(u)\cdot\nabla\varphi - \frac{1}{2}\epsilon\nabla\varphi\cdot\nabla\varphi && (37)
\end{aligned}
$$

is the enthalpy density.
At first glance, it seems physically adequate to calculate the energy release rate of (33) with respect to the crack length in order to formulate a Griffith fracture criterion [11]. However, the enthalpy functional is not convex and therefore the existence of an (unique) energy minimiser can mathematically not be guaranteed consistently that no unique weak solution of the EULER-LAGRANGE equations (30) exists.
In the following subsection we suggest a way out of these difficulties, namely to consider the positive definite part of the enthalpy.

4.3 The positive definite part of the enthalpy

The main idea presented in this paper is to delete the negative part of the enthalpy functional such that the remaining part is positive definite. Though, two of the five eigenvalues of the material matrix can be calculated without any problems (a positive and a negative one), the remaining three are not so easy to cope with. The representation of the remaining eigenvalues is quite complicated and it is hardly possible to determine generally whether they are positive or negative without inserting the material constants. To avoid this problem and to determine the negative part of the enthalpy, the SCHUR complement method is quite useful. Thus we get our main result:

Theorem 4.4. *Assume that the material constants $c_{11}, c_{33}, \epsilon_{33}$ and ϵ_{11} are positive; $C = c_{11}c_{33} - c_{13}^2 > 0$ and $B = c_{44} + \frac{e_{15}^2}{\epsilon_{11}} > 0$. Then the following simplified linear piezo-electric equation system generates a positive definite part of the enthalpy:*

$$
\begin{aligned}
\sigma &= c\varepsilon - eE && (38)\\
-E &= \epsilon^{-1}e\varepsilon. && (39)
\end{aligned}
$$

In particular, the positive definite part of the enthalpy conicides with the modified Helmholtz free energy:

$$
\begin{aligned}
E_{pos} &= \frac{1}{2}\int_{\Omega_\delta}(c\varepsilon\cdot\varepsilon + \epsilon\nabla\varphi\cdot\nabla\varphi)\,dx.\\
&\overset{(39)}{=} \frac{1}{2}\int_{\Omega_\delta}(c + e^\top\epsilon^{-1}e)\varepsilon\cdot\varepsilon\,dx. && (40)
\end{aligned}
$$

Proof. As the enthalpy density has a quadratic form and can be described in the matrix-vector form as

$$H = \frac{1}{2}\tilde{A}\mathcal{B}^*U^* \cdot \mathcal{B}^*U^*,$$

we write

$$\tilde{A}\mathcal{B}^*U^* = \begin{pmatrix} c & -e^T \\ -e & -\epsilon \end{pmatrix} \cdot \begin{pmatrix} \varepsilon(u) \\ -\nabla\varphi \end{pmatrix} = -F = -\begin{pmatrix} F_1 \\ F_2 \end{pmatrix}, \tag{41}$$

where

$$F_1 = \begin{pmatrix} f_{11} \\ f_{12} \\ f_{13} \end{pmatrix}, \qquad F_2 = \begin{pmatrix} f_{21} \\ f_{22} \end{pmatrix}.$$

Eliminating $\nabla\varphi$ from the second equation of (41) and inserting it into the first equation of (41) we get

$$\begin{aligned} \varepsilon(u) &= (c + e^T\epsilon^{-1}e)^{-1}(e^T\epsilon^{-1}F_2 - F_1), \\ \nabla\varphi &= \epsilon^{-1}[e(c + e^T\epsilon^{-1}e)^{-1}(e^T\epsilon^{-1}F_2 - F_1) - F_2]. \end{aligned}$$

Inserting the material matrices of the plane-strain state (13)

$$c = \begin{pmatrix} c_{11} & c_{13} & 0 \\ c_{13} & c_{33} & 0 \\ 0 & 0 & c_{44} \end{pmatrix}, \; e = \begin{pmatrix} 0 & 0 & e_{15} \\ e_{31} & e_{33} & 0 \end{pmatrix}, \; \epsilon = \begin{pmatrix} \epsilon_{11} & 0 \\ 0 & \epsilon_{33} \end{pmatrix},$$

into $\varepsilon(u)$ one gets

$$\varepsilon(u) = \frac{1}{J}\left[\begin{pmatrix} (c_{33}e_{31} - c_{13}e_{33})\frac{f_{22}}{\epsilon_{33}} \\ (c_{11}e_{33} - c_{13}e_{31})\frac{f_{22}}{\epsilon_{33}} \\ \frac{Je_{15}}{c_{44}+\frac{e_{15}^2}{\epsilon_{11}}}\frac{f_{21}}{\epsilon_{11}} \end{pmatrix} - \begin{pmatrix} (c_{33} + \frac{e_{33}^2}{\epsilon_{33}})f_{11} - (c_{13} + \frac{e_{31}e_{33}}{\epsilon_{33}})f_{12} \\ -(c_{13} + \frac{e_{31}e_{33}}{\epsilon_{33}})f_{11} + (c_{11} + \frac{e_{31}^2}{\epsilon_{33}})f_{12} \\ \frac{J}{c_{44}+\frac{e_{15}^2}{\epsilon_{11}}}f_{13} \end{pmatrix}\right]$$

where

$$J = (c_{11} + \frac{e_{31}^2}{\epsilon_{33}})(c_{33} + \frac{e_{33}^2}{\epsilon_{33}}) - (c_{13} + \frac{e_{31}e_{33}}{\epsilon_{33}})^2.$$

Furthermore,

$$\nabla\varphi = \frac{1}{J}\left[\underbrace{\begin{pmatrix} \frac{Je_{15}^2}{c_{44}+\frac{e_{15}^2}{\epsilon_{11}}}\frac{f_{21}}{\epsilon_{11}^2} \\ \left((c_{33}e_{31}^2 - 2c_{13}e_{33}e_{31} + c_{11}e_{33}^2)\right)\frac{f_{22}}{\epsilon_{33}^2} \end{pmatrix}}_{\varphi^*} - \begin{pmatrix} \frac{J}{c_{44}+\frac{e_{15}^2}{\epsilon_{11}}}\frac{e_{15}f_{13}}{\epsilon_{11}} \\ (c_{33}e_{31} - c_{13}e_{33})\frac{f_{11}}{\epsilon_{33}} + (c_{11}e_{33} - c_{13}e_{31})\frac{f_{12}}{\epsilon_{33}} \end{pmatrix}\right] - \begin{pmatrix} \frac{f_{21}}{\epsilon_{11}} \\ \frac{f_{22}}{\epsilon_{33}} \end{pmatrix}.$$

The enthalpy density (37) can be expressed by F_1, F_2 using the above relations for ε and $\nabla\varphi$. After longer straight forward calculations we get

$$\begin{aligned} H &= \frac{1}{2B}\left(\frac{e_{15}}{\epsilon_{11}}f_{21}-f_{13}\right)^2 \\ &+\frac{1}{2JK}\left(\frac{K}{\epsilon_{33}}f_{22}-((c_{33}e_{31}-c_{13}e_{33})f_{11}+(c_{11}e_{33}-c_{13}e_{31})f_{12})\right)^2 \\ &+\frac{1}{2K}\left(e_{33}f_{11}-e_{31}f_{12}\right)^2-\frac{1}{2}(\frac{f_{22}^2}{\epsilon_{33}}+\frac{f_{21}^2}{\epsilon_{11}}), \end{aligned} \tag{42}$$

where

$$K = c_{11}e_{33}^2 - 2c_{13}e_{31}e_{33} + c_{33}e_{31}^2.$$

Note that the constants K and J are positive due to the assumptions on the material parameters, which are indeed satisfied for real materials. Furthermore,

$$C + \frac{K}{\epsilon_{33}} = J. \tag{43}$$

The representation of the enthalpy density H by the quadratic form (42) shows that we get a positive definite part setting

$$\frac{1}{2}(\frac{f_{22}^2}{\epsilon_{33}}+\frac{f_{21}^2}{\epsilon_{11}}) = \frac{1}{2}\epsilon^{-1}F_2\cdot F_2 = 0 \tag{44}$$

We remark, that the remaining part is indeed positive definite due to the assumptions on the material parameters.

From (44) it follows that $F_2 = 0$ and finally

$$\nabla\varphi = \epsilon^{-1}(-F_2 + e\varepsilon) = \epsilon^{-1}e\varepsilon(u). \tag{45}$$

Thus, the constitutive relation (45) between mechanical strain and electric field strength has to be linear in order to guarantee positive definiteness. The field equations (38),(39) describe this situation. Finally, inserting (45) into the enthalpy density (2)

$$E_{enth} = \int_{\Omega_\delta} \frac{1}{2}c\varepsilon\cdot\varepsilon - \frac{1}{2}\epsilon\nabla\varphi\cdot\nabla\varphi + e\varepsilon\cdot\nabla\varphi\, dx.$$

we get E_{pos} defined by (40). □

Remark 4.5. Physically, the constitutive law (45) means to neglect higher order or back coupling effects, i.e. one assumes that electric loads which are induced by the piezoelectric effect will not reinduce mechanical displacements themselves and the other way round. Obviously, this model can only hold if electric potential and mechanical displacement are small enough such that the neglection of back coupling does not induce too big errors.

Now, we have to discuss in which appropriate function space a minimizer of E_{pos} exists, how the boundary value problem for the corresponding EULER-LAGARANGE equations look like and finally how to compute the energy release rate and to formulate a fracture criterium of Griffith‘s type.

5 The modified boundary value problem

As we have seen, in order to neglect the negative definite part of the enthalpy, we demand (45), that means

$$\nabla\varphi = \epsilon^{-1} e\varepsilon(u).$$

It follows, that the electric displacement field vanishes,

$$D = e\varepsilon - \epsilon\nabla\varphi = 0, \tag{46}$$

and the mechanical stress can be written as

$$\sigma = c\varepsilon + e^\top\nabla\varphi = c\varepsilon + \epsilon^{-1}e\varepsilon = (c + e^\top\epsilon^{-1}e)\varepsilon(u). \tag{47}$$

Introducing the material matrix $\tilde{c} = (c + e^\top\epsilon^{-1}e)$ we get a modified elastic HOOKE's law for the modified stress $\tilde{\sigma}$,

$$\tilde{\sigma} = \tilde{c}\varepsilon(\tilde{u}). \tag{48}$$

Here is

$$\tilde{c} = \begin{pmatrix} c_{11} + \frac{e_{31}^2}{\epsilon_{33}} & c_{13} + \frac{e_{31}e_{33}}{\epsilon_{33}} & 0 \\ c_{13} + \frac{e_{31}e_{33}}{\epsilon_{33}} & c_{33} + \frac{e_{33}^2}{\epsilon_{33}} & 0 \\ 0 & 0 & c_{44} + \frac{e_{15}^2}{\epsilon_{11}} \end{pmatrix} \tag{49}$$

The entrees of $\tilde{c}$, $c_{ij}[10^9\frac{N}{m^2}]$, $e_{ij}[10^9\frac{nC}{m^2}]$, $\epsilon_{ij}[10^9\frac{(nC)^2}{Nm^2}]$, are chosen

for PZT-4

$c_{11} = 23.8$	$e_{31} = -0.13$	$\epsilon_{11} = 0.110625$
$c_{33} = 10.6$	$e_{33} = 0.28$	$\epsilon_{33} = 0.106023$
$c_{13} = 2.19$	$e_{15} = 0.01$	
$c_{44} = 2.15$		

for BaTiO_3

$c_{11} = 166$	$e_{31} = -4.4$	$\epsilon_{11} = 11.2$
$c_{33} = 162$	$e_{33} = 18.6$	$\epsilon_{33} = 12.6$
$c_{13} = 78$	$e_{15} = 11.6$	
$c_{44} = 43$		

Now we discuss how we can derive from the original boundary value problem (17,..,22) a modified coupled boundary value problem such that (45) holds.

5.1 Reformulation of the boundary value problem

Let us repeat the original boundary value problem. Let Ω_δ be the cracked domain given in Figure 3.

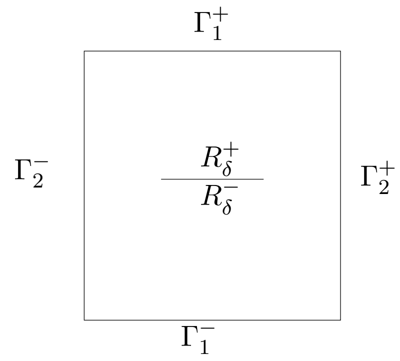

Figure 3: The cracked domain Ω_δ

Find the mechanical displacement field u and the electric potential field φ, such that

$$-\mathrm{Div}^\top \sigma = 0 \quad \text{in } \Omega_\delta, \quad \sigma = c\varepsilon + e^\top \nabla\varphi \tag{50}$$

$$\mathrm{div}\, D = 0 \quad \text{in } \Omega_\delta, \quad D = e\varepsilon - \epsilon\nabla\varphi \tag{51}$$

$$u = 0 \quad \text{on } \Gamma_1^- \tag{52}$$

$$\varphi = +\varphi_a \text{ on } \Gamma_1^+ \tag{53}$$

$$\varphi = -\varphi_a \text{ on } \Gamma_1^- \tag{54}$$

$$\sigma_n = N^\top \left(c\varepsilon(u) + e^\top \nabla\varphi\right) = 0 \quad \text{on } \Gamma_1^+ \cup \Gamma_2^\pm \cup R_\delta^\pm \tag{55}$$

$$D_n = n^\top (e\varepsilon(u) - \epsilon\nabla\varphi) = 0 \quad \text{on } \Gamma_2^\pm \cup R_\delta^\pm. \tag{56}$$

with

$$\mathrm{Div} = \begin{pmatrix} \partial_{x_1} & 0 \\ 0 & \partial_{x_3} \\ \partial_{x_3} & \partial_{x_1} \end{pmatrix}, \quad \sigma = \begin{pmatrix} \sigma_{11} \\ \sigma_{33} \\ \sigma_{13} \end{pmatrix}, \quad \varepsilon = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{33} \\ 2\varepsilon_{13} \end{pmatrix}.$$

Lemma 5.1. *Assume that $\varepsilon_{11} = 0$ on $\Gamma_1^+ \cup R_\delta^\pm \cup \Gamma_2^\pm$. Then the mechanical problem (50,52,55) for the modified model with $D = e\varepsilon - \epsilon\nabla\varphi = 0$ reads: Find $\tilde{u}$ such that*

$$-Div^\top \tilde{\sigma} = 0 \quad in\ \Omega_\delta, \quad \tilde{\sigma} = \tilde{\sigma}(\tilde{u}) = \tilde{c}\varepsilon(\tilde{u}) \tag{57}$$

$$\tilde{u} = 0 \quad on\ \Gamma_1^- \tag{58}$$

$$N^\top \tilde{\sigma} = A_1 \nabla\varphi \quad on\ \Gamma_1^+ \cup R_\delta^- \tag{59}$$

$$N^\top \tilde{\sigma} = -A_1 \nabla\varphi \ on\ R_\delta^+ \tag{60}$$

$$N^\top \tilde{\sigma} = \pm A_2 \nabla\varphi \ on\ \Gamma_2^\pm, \tag{61}$$

where

$$A_1 = \begin{pmatrix} \frac{c_{44}\epsilon_{11}}{e_{15}} + e_{15} & 0 \\ 0 & \frac{c_{33}\epsilon_{33}}{e_{33}} + e_{33} \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & \frac{c_{13}\epsilon_{33}}{e_{33}} + e_{13} \\ \frac{c_{44}\epsilon_{11}}{e_{15}} + e_{15} & 0 \end{pmatrix}.$$

Proof. We have to verify (59,60,61).
i) The boundary conditions on $\Gamma_1^+ \cup R_\delta^-$.
On these boundary pieces the normal vector is $n = (0,1)^\top$ and

$$N^\top \tilde{\sigma} = \begin{pmatrix} n_1 & 0 & n_3 \\ 0 & n_3 & n_1 \end{pmatrix} \begin{pmatrix} \tilde{\sigma}_{11} \\ \tilde{\sigma}_{33} \\ \tilde{\sigma}_{13} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \tilde{\sigma}_{11} \\ \tilde{\sigma}_{33} \\ \tilde{\sigma}_{13} \end{pmatrix} = \begin{pmatrix} \tilde{\sigma}_{13} \\ \tilde{\sigma}_{33} \end{pmatrix}.$$

Due to (48) and (49) we get

$$\begin{aligned} \tilde{\sigma}_{13} &= 2\tilde{c_{33}}\varepsilon_{13}, && (62) \\ \tilde{\sigma}_{33} &= \tilde{c}_{21}\varepsilon_{11} + \tilde{c}_{22}\varepsilon_{33}. && (63) \end{aligned}$$

On the other hand, relation (45) implies

$$\nabla\varphi = \begin{pmatrix} \frac{\partial\varphi}{\partial x_1} \\ \frac{\partial\varphi}{\partial x_3} \end{pmatrix} = \begin{pmatrix} \frac{2e_{15}\varepsilon_{13}}{\epsilon_{11}} \\ \frac{e_{31}\varepsilon_{11}+e_{33}\varepsilon_{33}}{\epsilon_{33}} \end{pmatrix}.$$

Since we have assumed that ε_{11} vanishes on $\Gamma_1^+ \cup R_\delta^-$, we can express the strain components

$$\begin{aligned} 2\varepsilon_{13} &= \frac{\epsilon_{11}}{e_{15}}\frac{\partial\varphi}{\partial x_1}, \\ \varepsilon_{33} &= \frac{\epsilon_{33}}{e_{33}}\frac{\partial\varphi}{\partial x_3} \end{aligned}$$

and insert them into (62) and (63). Taking in account (49) the boundary condition (59) follows.
ii) The boundary conditions on R_δ^+.
Having in mind that the normal vector is $n = (0,-1)^\top$ we come to the boundary condition (60) analogously to the first case.
iii) The boundary conditions on $\Gamma_2^\pm$.
On the boundary pieces $\Gamma_2^\pm$ the corresponding normal vectors read $n^\pm = (0, \pm1)^\top$. Since

$$N^\top \tilde{\sigma} = \pm \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{\sigma}_{11} \\ \tilde{\sigma}_{33} \\ \tilde{\sigma}_{13} \end{pmatrix} = \pm \begin{pmatrix} \tilde{\sigma}_{11} \\ \tilde{\sigma}_{13} \end{pmatrix}.$$

we can proceed as in the first case and the boundary condition (61) follows. □

Remark 5.2. The assumption that ε_{11} vanishes on $\Gamma_1^+ \cup \Gamma_2^\pm \cup R_\delta^\pm$ seems to be meaningfull because the polarisation axis is in x_3-direction.

The electric relations (51),(53),(54),(56) can be rewritten with the help of (46),(48). The resulting boundary value problem reads:

Find an electric potential field φ, such that

$$\begin{aligned} -\mathrm{div}\,(\epsilon\nabla\varphi) &= -\mathrm{div}\,(e\varepsilon(\tilde{u})) = -\mathrm{div}\,(e\tilde{c}^{-1}\tilde{\sigma}(\tilde{u})) \quad \mathit{in}\ \Omega_\delta && (64) \\ \epsilon\nabla\varphi\cdot n &= e\varepsilon(\tilde{u})\cdot n = e\tilde{c}^{-1}\tilde{\sigma}(\tilde{u})\cdot n \quad \mathit{on}\ \Gamma_2^\pm \cup R_\delta^\pm && (65) \\ \varphi &= \pm\varphi_a \quad \mathit{on}\ \Gamma_1^\pm. && (66) \end{aligned}$$

5.2 An iterative procedure

We propose an iterative procedure in order to compute the solutions $\tilde{u}$ and φ of the coupled mechanical and electric systems, that means of the mechanical boundary value problem (57),(58),...,(61) and the electric boundary value problem (64),(65),(66). To this aim we write both problems in a weak form:

The mechanical problem P(mech)

Let $\mathcal{V}_m = \{\tilde{u} \in [H^1(\Omega_\delta)]^2 : \tilde{u} = 0 \text{ on } \Gamma_1^-\}$.

Find a mechanical displacement field $\tilde{u} \in \mathcal{V}_m$ *such that* $\forall \tilde{v} \in \mathcal{V}_m$

$$\begin{aligned} a_m(\tilde{u}, \tilde{v}) &= \int_{\Omega_\delta} \tilde{c}\varepsilon(\tilde{u}) \cdot \varepsilon(\tilde{v})\, dx \\ &= \int_{\Gamma_2^+} A_2 \nabla\varphi \cdot \tilde{v}\, ds - \int_{\Gamma_2^-} A_2 \nabla\varphi \cdot \tilde{v}\, ds - \int_{R_\delta^+} A_1 \nabla\varphi \cdot \tilde{v}\, ds + \int_{R_\delta^- \cup \Gamma_1^+} A_1 \nabla\varphi \cdot \tilde{v}\, ds. \end{aligned}$$

We have got this formulation in the same way as in section 4 by partial integration. Note, that due to KORN's inequality and the LAX-MILGRAM theorem a uniquely defined weak solution $\tilde{u}$ exists.

The electric problem P(el)

Let $\mathcal{V}_e = \{\varphi \in H^1(\Omega_\delta) : \varphi = 0 \text{ on } \Gamma_1^\pm\}$. We decompose $\varphi = \varphi_0 + w$, where w is a fixed extension of the bondary data $\varphi_a^\pm$ into Ω_δ. Thus we can take e.g. $w = \frac{-2\varphi_a}{h} x_3 + \varphi_a$, where h is the height of Ω_δ.

Find an electric potential field $\varphi_0 \in \mathcal{V}_e$ *such that* $\forall \psi \in \mathcal{V}_e$

$$\begin{aligned} a_e(\varphi_0, \psi) &= \int_{\Omega_\delta} \epsilon \nabla\varphi_0 \cdot \nabla\psi\, dx \\ &= -\int_{\Omega_\delta} \epsilon \nabla w \cdot \nabla\psi\, dx + \int_{\Omega_\delta} e\varepsilon(\tilde{u}) \cdot \nabla\psi\, dx. \end{aligned}$$

We remark that an uniquely defined solution φ_0 exists and therefore $\varphi = \varphi_0 + w$ is well defined.

The proposed iterative procedure reads:

1. step Start with $\varphi = \varphi_1 = w$.

2. step Solve P(mech) with the right hand sides generated by φ_1 and denote the solution by $\tilde{u}_1$.

3. step Solve P(el) with the right hand sides generated by $\tilde{u}_1$ and denote the solution by $\varphi_2 = \varphi_{0,2} + w$.

4. step Go to step 2 and consider φ_2 instead of φ_1. Repeat the steps.

Remark 5.3. Until now, we have not proved that this iteration schema converges.

5.3 Energy release rate and the Griffith criterion

In elastic bodies GRIFFITH's fracture criterion describes in a quasistatic setting whether or not a preexisting crack will grow under external forces. It can be formulated in terms of the energy release rate (ERR) which is the derivative of the deformation energy with respect to a virtual crack extension.

Now we start from the problem P(mech). The corresponding deformation energy is defined for $\tilde{u}_\delta \in \mathcal{V}_m$ and a fixed $\varphi_\delta \in \mathcal{V}_e$:

$$I^m(\Omega_\delta) = I^m_\delta = \min\{I^m(\Omega_\delta, \tilde{u}_\delta); \tilde{u}_\delta \in \mathcal{V}_m\} = \min_{\tilde{u}_\delta}\{\frac{1}{2}\int_{\Omega_\delta} \tilde{c}\varepsilon(\tilde{u}_\delta)\cdot\varepsilon(\tilde{u}_\delta)\,dx$$
$$-\int_{\Gamma_2^+} A_2\nabla\varphi_\delta\cdot\tilde{u}_\delta\,ds + \int_{\Gamma_2^-} A_2\nabla\varphi_\delta\cdot\tilde{u}_\delta\,ds + \int_{R_\delta^+} A_1\nabla\varphi_\delta\cdot\tilde{u}_\delta\,ds - \int_{R_\delta^-\cup\Gamma_1^+} A_1\nabla\varphi_\delta\cdot\tilde{u}_\delta\,ds.\} \tag{67}$$

We remark that φ_δ is the weak solution of P(el). Therefore, the above boundary integrals are well defined, at least in the sense of dual pairing of $\nabla\varphi_\delta|_{\Gamma_i} \in W^{\frac{1}{2}}(\Gamma_i)'$ and $\tilde{u}_\delta|_{\Gamma_i} \in W^{\frac{1}{2}}(\Gamma_i)$.

We remember that the the domain Ω_0 has a straight crack of the length l, whereas Ω_δ has a crack of the length $l+\delta$.

GRIFFITH' fracture criterion can be reformulated for our modified piezoelectric model:

The crack $R_0^\pm$ in Ω_0 is stationary under electric load, if the deformation energy, which would be released at a crack extension, is less than the energy (dissipative energy) which is needed to create the new surface.

The simplest case is to assume that the dissipative energy $D(\Omega_\delta)$ is proportional to the geometrical macroscopic crack surface, that means

$$D(\Omega_\delta) = 2\gamma(l+\delta).$$

Then we can express this fracture criterion as follows:

The crack is stationary if

$$I^m(\Omega_0) - I^m(\Omega_\delta) \le D(\Omega_\delta) - D(\Omega_0) = 2\gamma\delta.$$

The energy release rate is defined as

$$\mathrm{ERR}(\Omega_0) = \lim_{\delta\to 0}\frac{I^m(\Omega_0) - I^m(\Omega_\delta)}{\delta}. \tag{68}$$

Therefore, GRIFFITH's fracture criterion can also be expressed as:

The crack is stationary if

$$\mathrm{ERR}(\Omega_0) = -(\frac{\partial I^m(\Omega_\delta)}{\partial\delta})|_{\delta=0} \le 2\gamma. \tag{69}$$

Note that the weak solutions of P(mech) and P(el) in Ω_0 or Ω_δ realize I^m_0 or I^m_δ, respectively.

The energy release rate can be computed with the help of a path-integral or a volume-integral. A rigorous mathematical derivation of these quantities and computations will be done in a forthcoming paper.

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